Chemistry and Materials Science Directorate News

Providing scientific excellence and leadership that meets and anticipates the needs of the Laboratory's programs

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Inside This Issue

Message from the Associate Director

The Chemistry and Materials Science (CMS) Directorate managers and staff have been busy during the last few months developing what we hope will be a coherent, long-range strategic plan for CMS. This plan is aimed at ensuring that we fulfill our two governing principles as a directorate: (1) delivering on our commitments to the programs and (2) anticipating change and capitalizing on opportunities through excellence in science and technology (S&T).

The plan that we are developing is synergistic with the Laboratory's institutional long-range S&T plan and 10-year site plan. Our goal is to create and publish a CMS plan that will help each of you to better understand the strategic directions of the Laboratory and CMS so that you can contribute fully to the Laboratory, both today and in the future. The following is a preview of some of the thinking behind the

Continued on page 10 ➤

chemistry & materials science CMS

Corner on Science

CMS-Funded Student Bears Fruit: Longer Atomistic Simulations and New Colors from Shocked Photonic Crystals

A new method devised by researchers in the Chemistry and Chemical Engineering Division (CChED) enables shocks to be simulated at the atomistic scale for a time period that is about 1000 times longer than simulations using traditional methods.

The previous technique for creating atomistic simulations followed a growing system of atoms over a period of time. However, the computational power needed to simulate the system as it expanded quickly exceeded the available resources. Thus, traditional atomistic simulations were limited to time periods of about 10 ps.

The new method overcomes previous limitations by simulating a representative subsystem of atoms instead of the entire system. Through a combination of molecular dynamics and continuum mechanics, the new technique can apply forces to a subsystem and simulate shocks for time periods as long as 5 ns.

Simulations using the new method are accelerated by a factor as high as 10^8. In other words, atomistic simulations that would have previously required approximately 10 million years to run can now be completed in about a month—a significant time savings.

Graduate fellow Evan Reed (left) and CMS scientist Larry Fried.

With these longer atomistic simulations, CChED researchers can investigate the chemistry of high explosives (i.e., how they release energy) when they are shocked. Moreover, the new method can be used to examine the effects of shock on a wide variety of materials, making the technique highly versatile and useful for Laboratory programs.

This new simulation technique resulted from a collaboration between CMS scientist **Larry Fried**; **Evan Reed**,

Continued on page 11 ➤

Interview With...

Christine Hartmann-Siantar

As the director of the Laboratory's Glenn T. Seaborg Institute, **Christine Hartmann-Siantar** considers herself fortunate to have found a career where she can do what she loves—namely, apply science and technology to help people live happier, longer lives.

Christine grew up on a farm in Wisconsin and received a bachelor's degree in physics and a Ph.D. in medical physics from the University of Wisconsin, Madison. During her late undergraduate and early graduate career, Christine lost many family members to cancer. This experience kindled her lifelong interest in cancer treatment and influenced her decision to work in medical physics.

After completing a medical physics residency, Christine became a radiation physicist at the Medical College of Wisconsin, where she made sure that each cancer patient received the appropriate radiation dose for his or her treatment plan. Although Christine enjoyed her work, she decided to accept a Laboratory position that offered the possibility of helping cancer patients on a much larger scale.

Continued on page 11 ➤

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A PDF of this newsletter with clickable Web links can be downloaded from the CMS Web site: http://www-cms.llnl.gov/news/newsletter.html.

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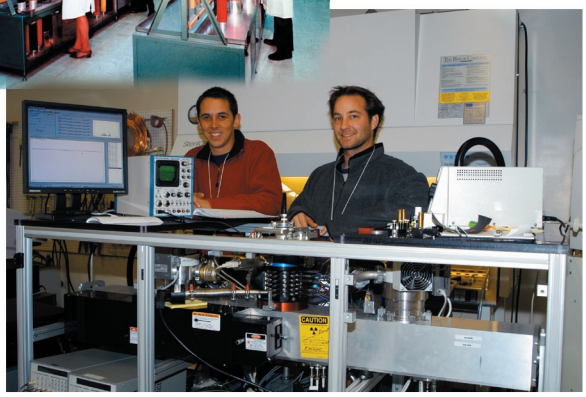
National Nuclear Security Administration

Directorate News

Revitalized Complex Serves CMS's National-Security Mission

BY DAVE SMITH

Room 1143 in Building 151 formerly serviced the gas diagnostics effort of the nuclear testing program and was outfitted with several racks of glass vacuum lines.



Within the past two years, Room 1143 has been completely renovated and now houses spectrometers and preparation areas for the bioaerosol mass spectrometry laboratory.

In November 2003, residents of the Building 151 complex (Buildings 151, 152, 154, and 155 and Trailer 1541) celebrated the end of an intensive period of structural retrofits and additions that brought Building 151 to modern seismic standards. As a newly outfitted national-security facility, the complex is ready to serve the defense, nonproliferation, and homeland security missions important to the Laboratory and the nation.

Building 151, a 100,000-sq.-ft. multiuse facility, was constructed in the late 1960s to support the nuclear testing program. The building contains high- and low-level radiochemistry laboratories; a radioactive solid-core dissolver wing; clean rooms; environmental- and wet-chemistry laboratories; analytical instrumentation and nuclear counting facilities; and secure work areas with adjoining, unclassified office space.

More space was needed as CMS's mission diversified during the 1990s and extended beyond traditional support to the nuclear weapons program. Building 154, a 10,000-sq.-ft., general-purpose laboratory facility, was designed and built in the early 1990s to support Livermore's nonproliferation and environmental-science missions. In 2003, Building 155 was constructed, adding 22,000 sq. ft. for classified and unclassified work and for a 150-seat auditorium.

The complex, which currently houses the staff and core scientific capabilities of the Chemical Biology and Nuclear Science Division, is configured so that research groups are collocated with their experimental facilities. For example, the second floor of Building 151 is primarily dedicated to sample characterization and analysis. Higher-level radiochemistry, nuclear forensic and attribution, and mass spectrometry laboratories occupy the first floor, and low-background counters and detectors reside in the basement.

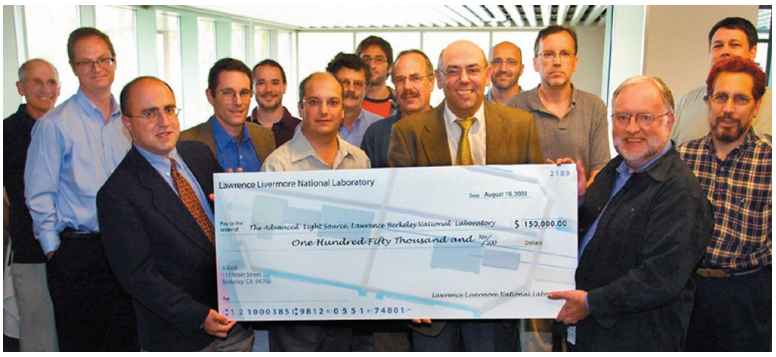
Buildings 151 and 154 also provide needed space for the specialized experimental needs of CMS programs and institutes. For instance, in Building 151, CMS Environmental Services inhabits the second floor; the first floor contains radiochemistry laboratories used by Stockpile Radiochemistry, an experimental center for bioaerosol mass spectrometry, and the main office of the Glenn T. Seaborg Institute; and the Center for National Security Applications of Magnetic Resonance houses five nuclear magnetic resonance spectrometers in the basement. Moreover, the BioSecurity and Nanosciences Laboratory occupies all of Building 154 and Trailer 1541.

The refurbished complex provides modern experimental facilities that link laboratories with both unclassified and secure data analysis centers, new levels of safety for building residents and neighbors, and room for future programmatic expansion. In addition, the collocation of experimenters from different disciplines fosters collaboration between the nuclear, chemical, and biological sciences. The newly renovated complex will enable CMS to continue to meet our national-security and scientific missions in the years to come. ■

CMS-Funded Membership Advances the Laboratory's High-Pressure Research Capabilities

With a $150,000 contribution from CMS on August 19, 2003, the Laboratory became a member of a high-pressure science consortium within the California High-Pressure Science Observatory (CALIPSO) program.

The CALIPSO program is currently focused on developing a new beamline at the Advanced Light Source, a synchrotron facility at the Lawrence Berkeley National Laboratory. As the first fully dedicated high-pressure and high-temperature synchrotron beamline on the West Coast, the new beamline will provide expanded experimental opportunities for CMS staff to conduct research on issues concerning extreme chemistry and synthesis, Earth and planetary science, nanomaterials, and energetic materials.



A symbolic check for $150,000 in support of the California High-Pressure Science Observatory program is given by CMS's Lou Terminello (front left) to team leaders at the Advanced Light Source.

Understanding chemistry under extreme pressure and temperature is a key challenge of the Laboratory's stockpile stewardship mission. The high-synchrotron brightness of CALIPSO will provide critically important research capabilities to CMS scientists by enabling them to rapidly collect phase, stability, chemical, kinetic, and structural information at high pressures (up to hundreds of gigapascals) and temperatures (up to thousands of kelvin). The data collected from CALIPSO will advance the predictive capabilities of the Laboratory's computational efforts.

By conducting experiments with the new beamline, CMS researchers hope to eventually find answers to technical questions regarding reaction chemistry, new states of matter, and planetary evolution. These experiments will further increase the reliability and performance of our country's national-defense systems.

To learn more about CALIPSO, Laboratory employees are encouraged to contact **Pat Allen** (allen42@llnl.gov), the deputy division leader, science and technology, for the Chemistry and Chemical Engineering Division (CChED), and CChED scientist **Joe Zaug** (zaug1@llnl.gov). ■

CMS Scientists Tackle Materials Problems in the Energy Programs

Workshop organizers (left to right): John Ziagos, Cindy Atkins-Duffin, and Ravi Upadhye.

A new workshop to discuss materials issues in the Laboratory's Energy programs was attended by approximately 40 scientists from the CMS and Energy & Environment (E&E) directorates on September 17, 2003.

The workshop was the brainchild of **Ravi Upadhye**, the CMS deputy materials program leader in E&E; **John Ziagos**, E&E's Energy Technology Division leader; and **Cindy Atkins-Duffin**, E&E's Energy Program leader at the time. While discussing materials problems in various Energy programs, the three scientists realized that these seemingly disjointed problems could be grouped under unifying themes. With the guidance of **Jeff Kass**, CMS's principal deputy associate director, the trio decided to organize a workshop where CMS and E&E scientists could share their materials problems and possible solution technologies.

During the first half of the workshop, principal investigators from E&E each provided an overview of a specific Energy program and the materials issues (e.g., stress corrosion cracking, high temperatures, radiation damage) encountered within that program. CMS researchers took the stage during the second half. Each CMS materials scientist discussed a current research technology (e.g., corrosion research, grain boundary engineering, high-temperature materials, surface science, new materials, sensors) that could be used to address a single materials issue across several Energy programs.

The workshop concluded by identifying specific research areas that would contribute the most to solving materials problems within the Energy programs. Since then, E&E and CMS have chosen to pursue external funding for research-and-development efforts in four main areas: conventional nuclear reactors, generation IV nuclear reactors, zero emissions steam technology, and solid-oxide electrolyzers and fuel cells.

CMS looks forward to continuing our strong partnership with E&E, and thanks Ravi, John, and Cindy for coming up with an innovative workshop that helps our two directorates share knowledge and devise solutions to scientific problems in the national interest. ■

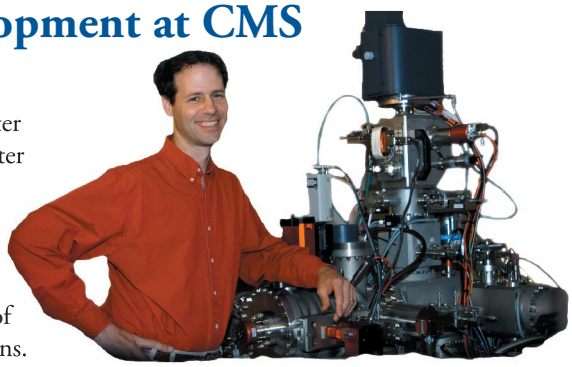
Laboratory Directed Research and Development at CMS

New Contributors to LDRD: Peter Weber

A Laboratory Directed Research and Development (LDRD) project provided **Peter Weber** with his first postdoctoral research position in April 2002. Peter is now a researcher in the Chemical Biology and Nuclear Science Division and the principal investigator of a promising, new LDRD endeavor, "Bioforensics: Attribution of biological weapons agents by NanoSIMS," an Exploratory Research in the Directorates project sponsored by CMS.

The need for a secondary-ion mass spectrometry (SIMS) instrument to conduct his dissertation research first brought Peter to Livermore in February 1998. Peter performed SIMS analyses in Building 154 with CMS scientist **Ian Hutcheon** and was later invited to participate in Ian's LDRD research as a postdoc in the Energy & Environment Directorate. After working with both Ian and CMS scientist **Christine Hartmann-Siantar**, Peter joined CMS in February 2003. Peter is now responsible for using the new NanoSIMS instrument, CMS's state-of-the-art ion probe machine, to acquire nanometer-scale, quantitative, in situ images of elemental and isotopic compositions.

Peter's LDRD project supports national security by developing a research technique that can potentially determine where, when, and how biological weapons (e.g., anthrax) were produced. Specifically, Peter and his colleagues will use the NanoSIMS to examine the spatial distribution of isotopes and trace elements in biological weapons spores (experiments will be conducted with an anthrax surrogate, not anthrax itself). This information is extremely valuable since the distribution of isotopes and trace elements varies depending on the processes used to produce the spores and when and where the spores were produced.



Peter Weber with the NanoSIMS, CMS's state-of-the-art ion probe machine.

Livermore's NanoSIMS is one of only ten instruments worldwide with the necessary sensitivity and spatial resolution—as small as 50 nm—to image isotopes and trace elements in biological weapons spores. Using the NanoSIMS will allow researchers to obtain information from very small samples and to analyze biological weapons spores separately from debris materials and other contaminants. ■

Postdoc News

Fall 2003 Off-Site Meeting

The CMS Postdoctoral Program fall off-site took place on October 27, 2003, at the Wente Vineyards Restaurant. Our guest speaker was **David Ashley**, executive vice chancellor and provost of UC Merced.

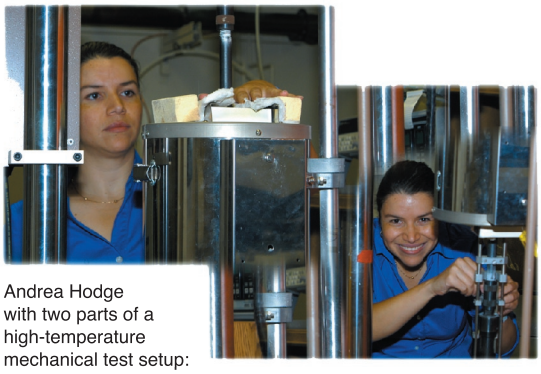
Postdoc People News

- Welcome to our new postdocs: **David Clatterbuck**, **Bassem El-Dasher**, **Marco Plomp**, and **Julie Smith**.
- Recent alumni of the Postdoctoral Program include **Olgica Bakajin**, **Christoph Bostedt**, **Julio Camarero**, and **Jenny Heidbrink**. We wish them luck. ■

Postdoc Profile: Andrea Hodge

During the 1994 World Cup season, CMS postdoc **Andrea Hodge** looked for a summer class that would give her time to cheer on the South American teams. An avid soccer fan from Colombia studying mechanical engineering at the University of Nevada, Las Vegas, Andrea chose introductory materials science, thinking that since it wasn't an engineering core class, she could skip lectures whenever her favorite teams played.

Much to her surprise, Andrea found materials science so interesting that she didn't miss a single class. Impressed by the field's ability to keep her attention, Andrea explored materials science research topics, eventually investigating the use of acoustic waves in nondestructive testing techniques for her senior design project. In 2002, Andrea received a Ph.D. in materials science and engineering from Northwestern University, where her dissertation focused on the processing of intermetallic foams and their high-temperature behavior.



Andrea Hodge with two parts of a high-temperature mechanical test setup: a furnace (left) and an extensometer (right).

Andrea was introduced to the Laboratory by her graduate school friend **Chris Schuh**, a former Lawrence fellow. Andrea joined CMS in July 2002 and works in the Materials Science and Technology Division's Stockpile Metallurgy Group with **Gil Gallegos**, **T.G. Nieh**, and **Luke Hsiung**. Her current projects include examining the nanomechanics of nanocrystalline and amorphous materials and the high-temperature properties of ultrafine

Continued on page 5 ➤

Notable Publications BY MICHAEL FLUSS

Scientific Communication—Highlighting Research Topics Important to the Laboratory Mission

An important part of the scientific endeavor is sharing ideas and discoveries with the entire community. This issue's Notable Publications section highlights three CMS scientists, **Jim Tobin**, **Randy Simpson**, and **Vasily Bulatov**, who have generated interest in research topics of importance to the Laboratory by either organizing research symposia at professional conferences or by publishing thought-provoking journal articles.

Research Symposia

At the 2003 Materials Research Society (MRS) Fall Meeting, CMS scientists helped organize research symposia on actinides and energetic nanomaterials, two topics of interest to the Laboratory. Both symposia facilitated an extraordinary exchange of ideas among top scientists and provided public exposure for many Livermore ideas and innovations. The proceedings for each symposium will be published as part of the MRS Symposium Proceedings Series, which can be viewed by MRS members at http://www.mrs.org/publications/epubs/proceedings/fall2003/.

Jim, a scientist in the Materials Science and Technology Division (MSTD), cochaired "Actinides: Basic science, applications, and technology," a three-day symposium with sessions on actinide phase stability, transformations, and aging; phononic and electronic structure; actinides and the environment; actinide solution and interfacial chemistry; the theory of actinides; and superconductivity, correlated behavior, and quantum criticality. The many superb speakers included MSTD scientists **Luke Hsiung**, **Kerri Blobaum**, **Brandon Chung**, **Joe Wong**, **Kevin Moore**, and **Babak Sadigh**, as well as international experts such as **Gerry Lander**, the director of the Institute for Transuranium Elements in Germany.

The second symposium, "Synthesis, characterization, and properties of energetic/reactive nanomaterials, featured a technical session that was co-organized by Randy, the leader of the Chemistry and Chemical Engineering Division (CChED). During this session, noteworthy research findings on sol-gel-derived energetic nanostructures were presented by CChED scientists **Alex Gash** and **Brady Clapsaddle**. They highlighted *proton scavenging*, a CMS-developed sol-gel chemistry technique that can be used to create nanostructured metal oxides and mixed metal oxides from most transition and lanthanide series elements. The symposium resulted in useful feedback for our scientists and in an exchange of new technical results in the nanoscience area of energetic materials.

Vasily Bulatov

Research Journal Articles

Vasily, a leader in computational materials science, is developing new formalistic principles and mathematical methods to predict the dynamic properties of materials, a topic of great relevance to Livermore programs. Vasily helped write two review articles in the *Journal of Computer-Aided Materials Design*. He also collaborated on a 2003 *Physical Review Letters* article that describes an interesting theoretical discovery.

Both review articles address the role of dislocations in dynamics. In the first paper, Vasily discusses recent developments and applications of dislocation dynamics methodology and their relevance to the dynamics of metals effort at the Laboratory and at other institutions. In the accompanying article, Vasily teams up with other Livermore and university experts to review recent research on the atomistic simulation of dislocation and defect properties of materials. This research is relevant to the multiscale modeling of plasticity and strength, with an emphasis on body-centered cubic metals and materials at extreme conditions.

The *Physical Review Letters* article, written by **Maurice de Koning**, **Wei Cai**, and Vasily, reports direct atomistic simulations of dislocation multiplication in face-centered cubic aluminum. These simulations revealed an unexpected mechanism, in which a Frank–Read source emits dislocations with Burgers vectors that are different from the source's Burgers vector. The researchers traced the mechanism to a spontaneous nucleation of partial dislocation loops within the stacking fault. The ability shown in this notable publication to discover a new mechanism and understand its origin will help guide future research in the materials dynamics field.

Publication Information and URLs

Bulatov, V. V. Current developments and trends in dislocation dynamics. *J. Comput.-Aided Mater.* **9**, 133 (2002). Available at http://journals.kluweronline.com/article.asp?PIPS=5141364.

de Koning, M., W. Cai, and V. V. Bulatov. Anomalous dislocation multiplication in fcc metals. *Phys. Rev. Lett.* **91**, 25503 (2003). Available at http://link.aps.org/abstract/PRL/v91/e025503.

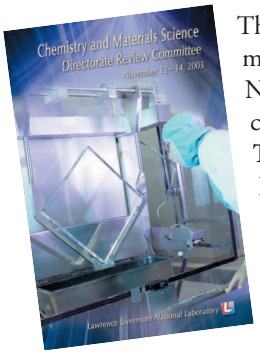
Moriarty, J. A., V. Vitek, V. V. Bulatov, and S. Yip. Atomistic simulations of dislocations and defects. *J. Comput.-Aided Mater.* **9**, 99 (2002). Available at http://journals.kluweronline.com/article.asp?PIPS=5141365. ■

Postdoc Profile: Andrea Hodge
Continued from page 4

lamellar titanium aluminides. In addition, as the CMS postdoc liaison, Andrea organizes the monthly postdoc seminars and invites guest speakers.

As an experimentalist, Andrea says that the Laboratory's extensive resources are like a dream, enabling her to study a variety of materials and test them in many ways. Andrea also enjoys working with others in CMS—her supervisors, who willingly share their knowledge; the other postdocs, who challenge her to be a better researcher and to write more papers; and the summer students, whom she loves to teach and advise. ■

November DRC Grades CMS as "Outstanding" BY JEFF KASS

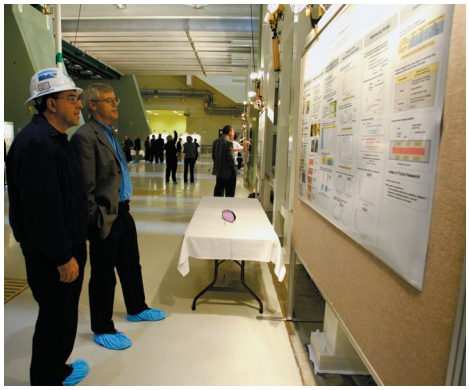


The CMS Directorate Review Committee (DRC) met at the National Ignition Facility (NIF) from November 12 to 14, 2003, to review CMS contributions to NIF. The DRC is chaired by **Tom Tombrello**, a professor at the California Institute of Technology, and draws its distinguished members from academic institutions and industry. With compliments for every talk and poster, the DRC again gave CMS "outstanding" grades for our scientific contributions, support to the NIF construction project, and efforts to make optimal use of scientific facilities and to recruit and retain a superb workforce.

Introductory Session

Following introductory remarks from Laboratory Director **Michael Anastasio**, several presentations explained NIF's importance to the Laboratory and provided an overview of CMS contributions.

Tomás Díaz de la Rubia, the CMS associate director, provided an update of the status and strategic directions for our directorate. He emphasized the importance of successful high-energy-density science, strong life-science contributions to the Laboratory's biosecurity responsibility, and leadership to fully integrate high-performance computing and experiments. Tomás also noted the alignment of CMS's strategic themes with the Laboratory's institutional strategy.



NIF Project Manager Ed Moses (left) and Jack Campbell.

George Miller, associate director for NIF Programs, described the central importance of NIF to the Laboratory's science and national-security mission. He highlighted recent successes, such as NIF early light, and advances in inertial confinement fusion (ICF) and stockpile stewardship that will be achieved as NIF becomes fully operational.

Ed Moses, **Craig Wuest**, **Trish Baisden**, **Jeff Atherton**, and **Jack Campbell** led an excellent tour through NIF, including the laser bays and the target chamber areas.

Terry Land (right) with DRC member Clyde Briant from Brown University.

John Lindl described the fundamental physics requirements for ICF, as well as resulting challenges in target fabrication.

Trish Baisden gave an overview of CMS support to NIF. Beginning with a history of laser science at Livermore, Trish described CMS efforts in targets and in materials problems that have been addressed for ICF optics. She also summarized research-and-development (R&D) efforts in potassium dihydrogen phosphate (KDP) and deuterated KDP (DKDP) glass to increase quality and output.

NIF Large Optics and Optical Materials

Presentations

Jack Campbell provided an overview of NIF optical-materials needs, laser amplifier glass, and KDP crystal fabrication. Jack described how the Laboratory develops large-area components and then transfers processes (e.g., optical blank fabrication, optical finishing, and coating deposition) to industrial partners.

Jeff Atherton highlighted the many beam path infrastructure challenges that have been overcome, including positioning multiton components with millimeter precision and maintaining unusually high cleanliness standards.

Bill Gourdin described efforts to solve and catalog nonoptical-materials issues.

Tayyeb Suratwala detailed brittle fracture R&D for improving the yield and lifetimes of NIF optics. Three cases were discussed in detail: indentation fracture of laser glass by mechanical support, impact fracture of the debris shield, and fracture by induced thermal stress during boule removal.

Posters

Ruth Hawley-Fedder highlighted the impurities and rapid growth of KDP and DKDP. She described a series of experiments exploring the effects of aluminum ions and ethylenediaminetetraacetic acid (EDTA) on KDP and DKDP growth.

Terry Land described the "virtual crystallizer," which uses mass transfer and kinetics and has successfully predicted the eventual shape and size of a KDP crystal.

Rebecca Dylla-Spears showed a mass transport model of KDP crystal growth. The model uses computational fluid dynamics. Future work will optimize rotation rates and patterns to control crystal shape and minimize inclusions.

Paul Ehrmann highlighted weathering tests of the phosphate glass slabs used in NIF. Weathering causes surface scatter that reduces the optic's transmission. A model was developed to calculate the degree of weathering with time and humidity.

Tien Shen described efforts to solve adhesion failures in the silver coating of aluminum flash lamp reflectors. Ways to prevent future such problems were identified.

Trish Baisden explained how NIF's 2ω laser will enhance stockpile stewardship and ICF, provide more energy on target, and enable experiments that scale strongly with energy.

Advanced Optical Materials and Fabrication Technologies

Jack Campbell gave an overview of advanced optical materials technologies. He highlighted large-crystal growth, specialized and complex optical component form fabrication, and

advanced methods for surface finishing.

Joe Menapace described the magnetorheological finishing and deterministic finishing of continuous-phase plates. A new method that carves a flat-topped pattern into phase plates has led to a continuous-phase plate fabrication process.

Rebecca Dylla-Spears (right) with DRC member Linda Trocki (far left) from Bechtel and former Lasers Associate Director John Emmett.

Pam Whitman summarized work on disposable debris shields to protect optics against soft x rays, shrapnel, and vaporized target debris. Pam identified a relatively inexpensive glass and ways to finish the glass and to achieve high-quality transmission of the laser wave front.

Jerry Britten described the development of large-aperture gratings for high-energy, short-pulse laser systems. The large-aperture grating development facility is a unique world-leading resource for large-area diffractive optics. Current efforts are directed toward fabricating a high-efficiency multilayer dielectric grating with the 800-mm aperture size required for the NIF high-energy petawatt laser.

Ruth Hawley-Fedder reviewed the crystal growth issues involved in the KDP elements. High growth rates for KDP were achieved by applying knowledge about basic crystal growth phenomena in supersaturated solutions to growth tank design. Encouraging rapid growth in DKDP still presents a challenge.

A tour of the crystal growth area concluded this session.

Advanced Concepts and Special Topics

Presentations

Alex Hamza provided an overview of the Nanoscale Synthesis and Characterization Laboratory. Advances in nanoscience will provide solutions for materials-driven, Laboratory-wide programmatic issues, with an initial focus on NIF targets. Success requires linked materials and engineering efforts.

Wayne King described the dynamic transmission electron microscope. The projected time and spatial resolution of this tool will open an experimental investigation regime for studying dynamic materials properties in unprecedented detail.

Wayne King (left) with DRC member Clyde Briant.

Posters

The final session included six posters covering quality assurance, target diagnostics, and target fabrication.

Chris Choate highlighted a sophisticated quality-control system that covers all components assembled into a line replaceable unit (LRU) and the LRU itself. This system includes a database of all data on both LRU components and complete LRUs.

Phil Miller described the investigation of a haze problem on the neodymium-doped phosphate glass slabs used in NIF. The problem was identified as residual polishing slurry, and aggressive, immediate postpolish cleaning was found to be an effective solution. Because of the rapid problem resolution, only a small number of amplifier slabs had to be returned for repolishing.

Greg Schmid detailed chemical vapor deposition (CVD) diamond stability issues for NIF operation. These issues are being addressed by radiation pumping the detectors as a preconditioning process that fills all available traps, allowing the detector's intrinsic performance to be realized. Saturation effects are addressed through detector geometry considerations. Synthetic single-crystal diamond detectors are also being explored.

Steve Letts showed the development of vapor-deposited polyamide ablator coatings for NIF ICF capsules. The process has been refined to meet the NIF specifications for surface roughness—a substantial accomplishment. Future work will improve our understanding of the solvent–vapor smoothing process and extend the method to other polymer systems.

Mitch Anthematten described the physics and phenomenology of solvent–vapor smoothing. The Laboratory has found a way to smooth surfaces through solvent–vapor exposures to dimethyl sulfoxide entrained in nitrogen. Mitch presented a model that accurately predicts behavior.

Joe Satcher's poster on the synthesis mechanisms of nanocellular materials completed the review. This new project will synthesize nanoporous metals (less than 10% full-density metals with pores measuring less than 500 nm) for use as laser targets in NIF high-energy-density science experiments. Recent work has revealed a gel formation mechanism, enabling the synthesis of metal (high-Z) oxide aerogels. These materials are needed to achieve the opacity required in radiation–hydrodynamics experiments and in ignition capsules. ■

Ruth Hawley-Fedder (right) with Pat Allen (far left), Terry Land, and John Emmett.

Awards and Personnel News

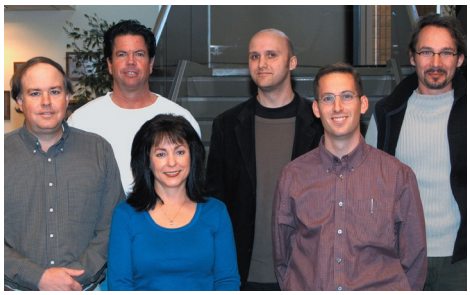
CMS Scientists Honored for Scientific Achievements and Leadership

CMS proudly announces the following honors recognizing our employees' scientific achievements and leadership:

- The American Ceramics Society gave the George W. Morey Award to CMS senior scientist **Jack Campbell**, the group leader for Advanced Optical Materials at the National Ignition Facility. Jack was honored for his "work and leadership in the development, characterization, and manufacturability of phosphate laser glass for high-peak power lasers."
- **David Eaglesham**, the CMS chief technologist, was elected vice president (president-elect) of the Materials Research Society, the world's leading forum for advanced, cutting-edge interdisciplinary materials research.
- **John Elmer**, the group leader for Materials Joining, was named a 2003 fellow of the American Society for Metals in recognition of his contributions to the use of synchrotron radiation in welding science. John's award cited his "development and application of synchrotron-based, in situ, spatially resolved x-ray diffraction techniques to permit quantitative understanding of phase transformation kinetics during fusion welding."
- CMS senior scientist **Joe Farmer** was selected as a member of the Defense Science Board (DSB) Task Force on Corrosion Control. The DSB's technical experts advise the Secretary of Defense on matters of interest to the Department of Defense.
- **Christian Mailhiot**, the division leader of the Materials Science and Technology Division, was elected a fellow of the American Physical Society (APS), an honor given to no more than 0.5% of the APS membership. Christian was nominated by APS's Division of Materials Physics for his "outstanding contributions and scientific leadership in theoretical and computational condensed matter and materials physics, with particular emphasis on innovative discoveries related to quantum-confined semiconductor structures and high-pressure research."
- CMS metallurgist **T.G. Nieh** was named a 2004 fellow of The Minerals, Metals & Materials Society (TMS) for his "contributions to the understanding of the superplasticity behavior of metals and ceramics, including high strain rate superplasticity and superplastic ceramics." No more than 100 of the nearly 10,000 TMS members can be living fellows.
- **Charlie Westbrook**, the CMS acting chief scientist, was elected vice president (president-elect) of the Combustion Institute, an international, scientific society that promotes and disseminates research in combustion science. ■

Welcome to the Directorate

We warmly welcome our CMS new hires, including **Olgica Bakajin** and **Julio Camarero**, who completed their Lawrence fellowships in October 2003 and are now CMS employees. ■



Clockwise from front left: CBND chemists **Michael Kristo**, **Norris "Kip" Harward**, and **Philip Wilk**; MSTD physicist **Juergen Biener**; CBND engineer **Joseph Tringe**; and CBND administrative specialist **Roseanne Kamerdula**. Not pictured: MSTD postdocs **Bassem El-Dasher** and **Erik Nelson**, CBND postdoc **Marco Plomp**, CMS engineer **Roger Rocha**, and CBND environmental scientist **Paul Spackman**.

So Long, Farewell, Good-Bye…

CMS bids a fond farewell to the following employees who have departed from our directorate. We thank them for their service to the Laboratory and wish them all the best!

Martyn Adamson, CChED chemist
Brian Andresen, AD staff chemist
Christoph Bostedt, MSTD postdoc
David Chambers, CBND chemist
Betty Cuevas, CChED administrative specialist
Arthur Denison, MSTD physicist
Dennis Fleming, MSTD senior technologist
Jerry Forbes, CChED physicist
Jeffrey Haas, CBND chemist
Carola Laue, CBND chemist
Simon Morton, MSTD postdoc
Boyd Taylor, CChED chemist ■

Making Us Proud: CMS Recipients of Directorate Awards

CMS Directorate Awards

Exceptional Service Awards

Ken Moody, **John Wild**, **Mark Stoyer**, **Nancy Stoyer**, and **Carola Laue**, discovery of the superheavy elements 114 and 116

T.G. Nieh, 2004 fellow of The Minerals, Metals & Materials Society

Distinguished Service Award

Jim Fischer, safety analysis program for nonnuclear hazards

Excellence in Publication Awards

Olgica Bakajin, "Single-molecule measurement of protein folding kinetics"

Joe Wong, **Dan Farber**, **Florent Occelli**, **Adam Schwartz**, **Mark Wall**, and **Carl Boro**, "Phonon dispersions of fcc δ-plutonium–gallium by inelastic x-ray scattering"

Awards from Other Directorates

Administration and Human Resources

Lori Turpin, special contribution to the LHire system

Lori Turpin and **Diana Bradbury**, contributions to the Integrated Performance and Pay Program

Chief Financial Officer

Edna Waller, **Theresa Healy**, **Nancy Schoendienst**, and **Craig Schoendienst**,

Continued on page 9 ➤

Facilities/Operations News

Meet the CMS Information Systems Team

The CMS Information Systems (IS) team, located in Trailer 1602, provides Macintosh, PC, and UNIX support for the more than 1200 desktop computer systems in CMS. The team is also responsible for network installation and connectivity, printer setup and service, computer security, and server administration for all personnel located in CMS facilities.

For assistance, call the CMS IS hotline at ext. 4-COMP (4-2667). Any request that is not resolved over the phone is recorded and assigned to an IS team member. The hotline receives about 2200 calls each month, so each request is prioritized based on the date/time received and level of urgency.

The 4-COMP hotline is staffed from 8 AM to 5 PM during the workweek. If you have a computer problem outside of these hours, call the hotline to leave a message or to learn the pager number of the IS team member on call. For desktop computer issues, you can also contact the Laboratory's computer helpline, ext. 4-HELP (4-4357).

Sheri Miner leads the IS team. The UNIX group (**Chris Smith**, **Teresa Kamakea**, **Ray Spence**, and **Terry Flickinger**) handles UNIX workstation and server issues, while the following team members support Macintosh and PC systems in specific CMS building complexes: Building 151 (**Karen Clendenin**, **Tony Hazlett**, and **John Wong**), Building 235 (**Jim Dilk**, **Lee Pittson**, and **George Williams**), and Building 132 (**Daphne Dugan**). **Fred Miller**, the primary information systems security officer; **Dawn Areson**, the network manager; **James Marriott**, the help desk coordinator; and intern **Sunny Woo** round out the team. ■

CMS Information Systems team members in the summer of 2003.

Making Us Proud

Continued from page 8

completion of the content and pilot program for financial management training

Defense and Nuclear Technologies

Geoff Campbell and **Vicki Mason-Reed**, "661" test

Jeff Colvin, laser-driven materials science

Karen Dodson and **Leonard Gray**, accomplishing programmatic long-term objectives

Larry Fried, excellence in communication of the Advanced Simulation and Computing (ASCI) Detonation Kinetics Program

Andrea Goins, processing 523 items for the Building 332 recovery lab in one year

Doug McAvoy, wall-to-wall inventory

Doug McAvoy and **Daniel Mew**, support during security condition (SECON) II

Daniel Mew, removal of transuranic waste drums

Daniel Mew and **Rich Torres**, analyses of spiked plutonium

John Molitoris and **Mike Howard**, Air Force Prompt Agent Defeat Program support

Robert Schmidt, joint actinide shock physics experimental research (JASPER) support

Energy & Environment

Victoria Dias, support of the Microbially Influenced Corrosion project

Ken Evans, technical excellence in developing a program for corrosion and electrochemical testing on the Yucca Mountain Program

Roger Grimm and **Dale Jones**, development of new stochastic analysis applications for intelligence information

Sharon Torres, bringing the capability of the scanning electron microscope imaging facilities to the Energy & Environment Directorate

Engineering

Brandon Chung and **Steve Thompson**, plutonium dilatometer activation

Karen Dodson, **Wendell Williams**, **Joseph Schmitz**, **Rich Torres**, **Daniel Mew**, **Bart Ebbinghaus**, and **Don Bajao**, accelerated aging alloy fabrication

Mark Lane, W80 surveillance support

Robert Maxwell, Center for National Security Applications of Magnetic Resonance

George Overturf, x ray computed tomography

Todd Palmer, **Mark Gauthier**, and **Randolph Pong**, standard container project

Joe Satcher and **Robert Maxwell**, silicon characterization

Nancy Schoendienst, Cost Accounts Funding Effort (CAFÉ) support

Leonard Summers, magnetohydrodynamic project

National Ignition Facility Programs

Jeff Atherton, **Jack Campbell**, **Jim Fair**, and **Tom Parham**, Laboratory's 50th Anniversary/Family Day

Lun Auyang, completion of the National Ignition Facility (NIF) amplifier blast shields

Chris Choate, Location Component and State Tracking System (LoCoS) restriction module

John Ertel, clean, dry air system for NIF

George Hampton, amplifier bus production and safety

Richard Meissner, nonvolatile residue test results

Tom Parham, contributions in support of NIF early light and first light

Nonproliferation, Arms Control, and International Security

Dan Archer, contributions to the engineering of a detection and tracking system for nuclear warfare defense at Fort Leonard Wood, Missouri

Howard Hall, support of a field test of radiation monitors under realistic conditions

Doug Manatt, expertise in data acquisition supporting the active interrogation of cargo

Physics and Advanced Technologies

Paul Mirkarimi, 2003 R&D 100 Award, "Ion beam thin film planarization"

Chris Walton, 2003 R&D 100 Award, "Extreme ultraviolet lithography full-field step-scan system"

Safety and Environmental Protection

Bryan Bandong, outstanding customer service ■

Message from the Associate Director
Continued from page 1

creation of this plan, particularly concerning its implementation. As you read, please keep in mind that this preview is not exhaustive; that is, it does not touch on all areas and priorities of the plan. Details regarding the areas of extreme chemistry and applied nuclear science will be provided in the near future.

Road Map to Implementation

I believe that a strategic plan is only as good as the road map that shows how to implement the plan. Given our expanding mission in a fiscally challenging environment, a clearly articulated road map is critical. We must define a limited set of the priorities that are essential for us to accelerate our progress across the entire spectrum of CMS missions. These priorities must be focused on the Laboratory's most pressing scientific and programmatic challenges and must be cross-cutting in the sense that successful execution will require partnerships with other directorates and collaborations with top academic institutions.

First, here are two crosscutting thrust areas that have emerged to guide the implementation of our strategic plan:

- Inorganic synthesis of novel materials and ultrafast characterization of dynamic phenomena in materials
- Molecular recognition chemistry and bioanalytical characterization and imaging

These two thrust areas are a key part of our road map's foundation. They show how to direct our resources to meet the Laboratory's evolving needs, specifically by ensuring the success of stockpile stewardship and high-energy-density (HED) science and of bioscience for national security and other Department of Energy (DOE) missions.

Our road map will help us to combine our directorate's principal currency of scientific exploration—namely, our people—with our world-class capabilities so that we can focus our investments on these two high-priority, mission-relevant thrust areas.

Our current budget constraints, which are forcing us to make difficult funding and hiring decisions, further underscore the need for careful implementation of these thrust areas if we wish to realize the full scientific and programmatic dividends of our investments.

Our directorate's involvement in the recent creation of the Nanoscale Synthesis and Characterization Laboratory (NSCL)—the highest priority item in the Stockpile Science and Technology section of the institutional long-range S&T plan—is the first step in implementing our strategic plan. We have redirected our internal resources (general and administrative, Laboratory-directed research and development, institutional general-purpose equipment, etc.) to fund the startup of this initiative, which is being formed in partnership with the Engineering, National Ignition Facility (NIF) Programs, and Defense and Nuclear Technologies directorates.

Our initial focus within NSCL will be to meet the S&T challenges posed by the targets that will be required for HED and inertial confinement fusion (ICF) experiments. In addition, we have started to pursue the development of some innovative electron-based diagnostics that can be used to investigate phase transitions and dynamics in materials under extreme conditions (e.g., temperatures, pressures, and strain rates).

We believe that these investments will lead to new ways of investigating materials and chemical reactions in time scales of hundreds of femtoseconds and length scales of nanometers. These possibilities are both scientifically exciting and programmatically relevant to our mission interests and will lead to further, significant investments in these two areas of materials science and chemistry.

The Laboratory's role in the nonproliferation of weapons of mass destruction and in homeland security continues to grow. As a discipline directorate, we have a strong role to play in ensuring the success of these programs, both today and in the future. Our strategic plan identifies these challenges and will provide a clear road map for prioritizing our investments in these areas.

For example, innovation in chemical and biological sensing, as well as radiation detection, is a grand challenge for the future. In addition, DOE plans to meet its mission in environmental microbiology through the creation of the Genomes to Life (GTL) program. These congressionally funded programs will lay the foundation for fundamental bioscience at the national laboratories in the 21st century. Livermore is a part of this vision, and CMS has an unambiguous role to play as both a partner and a technology provider to the Biology and Biotechnology Research Program. Finally, our employees in the BioSecurity and Nanosciences Laboratory and in the Glenn T. Seaborg Institute will lead the way in implementing Livermore's scientific initiatives in the areas of bioscience for national security and GTL. ■

CMS Strategic Plan

Crosscutting Thrust Area **Inorganic synthesis of novel materials and ultrafast characterization of dynamic phenomena in materials**	
Scientific Initiatives	Design and synthesis of novel materials for high-energy-density and inertial confinement fusion (ICF) targets
	In situ, real-time investigation of complex transient phenomena
University Alliances	*The Ultrafast Diagnostics Alliance* (W. King): UC Davis, University of Illinois at Chicago, University of Illinois at Urbana-Champaign, Florida State University, University of Michigan, Technische Universität (TU) Berlin, Arizona State University… *Lawrence Berkeley National Laboratory* (Advanced Light Source): R. Jeanloz et al.
LLNL Integration	Nanoscale Synthesis and Characterization Laboratory, ICF, H Division, Defense and Nuclear Technologies, Center for Micro and Nano Technology, Energetic Materials Center, Precision Materials Characterization Laboratory

Crosscutting Thrust Area **Molecular recognition chemistry and bioanalytical characterization and imaging**	
Scientific Initiatives	Bio-organic synthesis and nanofabrication
	Biomolecular imaging and characterization
University Alliances	*The Alliance for Nanoscience* (D. Eaglesham): UC Berkeley, UC Santa Barbara, UCLA, California Institute of Technology. *The Institute for Collaborative Bioscience* (J. De Yoreo, D. Eaglesham): UC Santa Barbara, Massachusetts Institute of Technology, California Institute of Technology
LLNL Integration	BioSecurity and Nanosciences Laboratory, M Division, Center for Micro and Nano Technology, Biology and Biotechnology Research Program, Glenn T. Seaborg Institute, Forensic Science Center

LLNL Mission

Corner on Science

Continued from page 1

a graduate fellow cofunded by CMS's Energetic Materials Center (EMC) and the former Materials Research Institute (MRI); and **John Joannopoulos**, Evan's graduate advisor at the Massachusetts Institute of Technology.

Evan first came to the Laboratory as a summer student in 1998 while pursuing his undergraduate degree in physics at the California Institute of Technology. Thanks to the joint efforts of **Randy Simpson** and **Mike McElfresh**, in 2001, Evan was awarded a three-year graduate fellowship that assured his continued close interaction with CMS scientists by bringing him back to the Laboratory each summer and for a few weeks each winter.

During his EMC/MRI graduate fellowship, Evan also conducted groundbreaking work on the properties of shocked photonic crystals, which are systems with layers of materials.

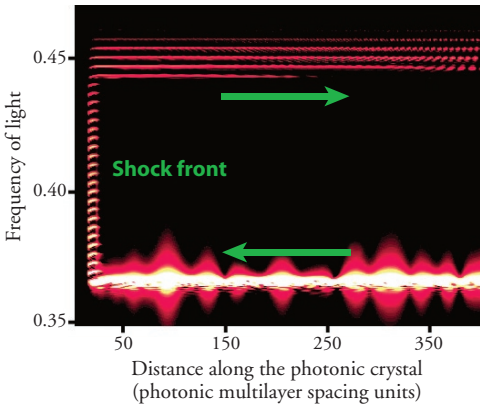


Fig. 1. Simulation of a shocked photonic crystal efficiently converting the frequency of light to a higher value. Light enters the crystal from the left (bottom arrow) and is reflected to the right by the shock (top arrow).

He discovered that sending a shock wave through a photonic crystal can convert the frequency of light (change its color) without losing energy (see Fig. 1). Furthermore, because each photonic-crystal layer has a unique refraction index for bending light, Evan realized that a photonic crystal can be "tuned" so that light is changed to a specific, desired frequency. The immense flexibility offered by tunable photonic crystals makes them possible replacements for the crystals currently used to convert light frequencies, such as the potassium dihydrogen phosphate (KDP) crystals in the National Ignition Facility.

Evan's work with shocked photonic crystals has been featured in *Nature*, *Physics Today*, ***New Scientist***, and *Science News*. CMS takes pride in the scientific accomplishments of Evan and other CChED researchers and looks forward to applying their theoretical work to the needs of Laboratory programs.

Related Publications

Reed, E. J. et al. Color of shock waves in photonic crystals. *Phys. Rev. Lett.* **90**, 203904 (2003). Available at http://link.aps.org/abstract/PRL/v90/e203904.

Reed, E. J. et al. A method for tractable dynamical studies of single and double shock compression. *Phys. Rev. Lett.* **90**, 235503 (2003). Available at http://link.aps.org/abstract/PRL/v90/e235503. ■

Interview With...

Continued from page 1

Thus, in 1993, Christine joined the research-and-development team of PEREGRINE, a project designed to improve cancer treatment by providing fast, affordable Monte Carlo simulations that model how different levels of radiation therapy will affect a patient's body. By using PEREGRINE, which was cleared for clinician use by the Food and Drug Administration in 2000, doctors can plan more accurate radiation treatments that maximize radiation dose to the tumor while minimizing damage to nearby healthy tissue. In recognition of her leadership and technical contributions to PEREGRINE, Christine was honored by the Laboratory with the prestigious Edward Teller Fellowship.

In 2001, Christine moved to CMS and became the director of the Seaborg Institute. She also serves at UC Davis as adjunct faculty in radiation oncology, a position that enables her to continue working with cancer patients. In addition, Christine meets regularly with UC Davis clinicians to gain feedback on the medical tools developed by the Laboratory.

Christine feels fortunate to be a part of CMS, which she describes as having a friendly atmosphere and as being very teamwork-oriented. She believes that at every level of the directorate, people are genuinely committed to doing their best for the country and to promoting outstanding science and technological innovation.

At the Seaborg Institute, Christine started a bionuclear initiative that combines nuclear science and technology with cutting-edge bioscience to serve societal needs. For example, researchers in the CMS and Biology and Biotechnology Research Program (BBRP) directorates are using nuclear science and molecular recognition to develop molecular-targeted radioisotope therapy, with the goal of improving the diagnosis and treatment of metastatic, or widespread, cancer. Current projects, led by **Rod Balhorn** and **Julie Perkins**, **Ian Hutcheon**, **Kai Vetter**, and **Peter Weber**, are developing molecular targeting agents and methods for imaging the presence of isotope-tagged molecules.

A separate bionuclear research area combines nuclear science and gene expression. For instance, the MINERVA project, which is a collaborative effort with researchers from UC Davis, Idaho National Engineering and Environmental Laboratory, and Montana State University, uses Monte Carlo simulations to obtain direct, in vivo samples of patient tissue exposed to radiation. In response to homeland security needs, other CMS scientists are working with **Andy Wyrobek's** BBRP research group to develop new ways of using gene and protein signatures to assess radiation dose after exposure. They are also investigating the possibility of making people temporarily resistant to radioactivity.

Christine is excited about the research being conducted at the Seaborg Institute. In the future, she hopes to extend radioactive tagging to questions about human behavior and cognition, such as exploring the biochemistry of creativity. ■

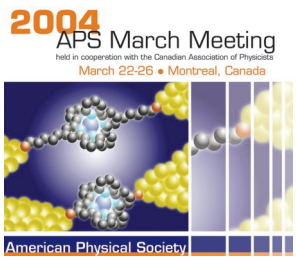
Conference Calendar

DATE	CONFERENCE	LOCATION	WEB SITE
January 7–9, 2004	2nd International Workshop, Multiscale Modeling of Strength and Fracture: Linking through the Mesoscale	Berkeley, CA	http://www-cms.llnl.gov/multiscale/
March 22–26, 2004	American Physical Society March Meeting 2004	Montreal, Canada	http://www.aps.org/meet/MAR04/
March 28–April 1, 2004	227th American Chemical Society National Meeting	Anaheim, CA	http://www.chemistry.org/portal/a/c/s/1/acsdisplay.html?DOC=meetings\anaheim2004\index.html
April 12–16, 2004	2004 Materials Research Society Spring Meeting	San Francisco, CA	http://www.mrs.org/meetings/spring2004/

Multiscale Modeling of Strength and Fracture: Linking through the Mesoscale

Participants at the Laboratory-sponsored 2nd International Workshop, Multiscale Modeling of Strength and Fracture: Linking through the Mesoscale, will discuss applying materials modeling to strength, fracture, and failure phenomena over a range of physical scales, with a special focus on modeling material deformation on the mesoscale. **Vasily Bulatov**, a materials physicist in the Materials Science and Technology Division (MSTD), is one of five workshop organizers and the primary technical contact.

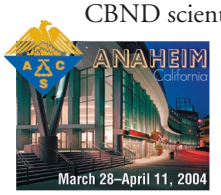
American Physical Society March Meeting 2004



The March 2004 meeting of the American Physical Society will feature two symposia organized by CMS scientists. **Riad Manaa**, a scientist in the Chemistry and Chemical Engineering Division, is co-organizing a symposium called "Simulations of matter at extreme conditions," while **Thomas Huser,** a researcher in the Chemical Biology and Nuclear Science Division (CBND) is co-organizing a symposium on "Nanoparticle-enhanced spectroscopies."

Please send items for the next newsletter (e.g., directorate news, awards, conference calendar items) to **Stephanie Shang** (shang2@llnl.gov).

227th American Chemical Society National Meeting



CBND scientists are organizing three symposia at the 227th American Chemical Society National Meeting. **Annie Kersting** is co-organizing a symposium on "Colloid-facilitated transport of contaminants in the subsurface: The life and death of a colloid." **John Reynolds** and **Brad Hart** are co-organizing a "Polymers and materials for antiterrorism and homeland defense" symposium, and **Aleksandr Noy** is co-organizing a symposium on "Nanoscale probing of intermolecular interactions."

2004 Materials Research Society Spring Meeting

As one of four cochairs of the 2004 Materials Research Society (MRS) Spring Meeting, **Jim De Yoreo**, the acting director of the BioSecurity and Nanosciences Laboratory, is co-organizing a "Frontiers of materials research" symposium. MSTD scientist **Mukul Kumar** is co-organizing a symposium called "Interfacial engineering for optimized properties," while CBND scientist **Sonia Létant** is co-organizing "Hybrid biological–inorganic interfaces." Other CBND researchers will be speaking at MRS symposia: **Julio Camarero** at "Proteins as materials;" **Chad Talley** at "Applications of novel luminescent probes in life science," a symposium co-organized by **Thomas Huser**; and **Jane Bearinger** at the "Biological and bio-inspired materials and devices" symposium, which is being co-organized by **Chris Orme**. In addition, MSTD scientist **T.G. Nieh** has been invited to speak at "Nanoscale materials and modeling—relations among processing, microstructure, and mechanical properties." ■

A PDF of this newsletter with clickable Web links can be downloaded from the CMS Web site: http://www-cms.llnl.gov/news/newsletter.html.